What is claimed is:

1. A method for designing a metal ion for use in a molecular dynamics simulation comprising the steps of:

a) building a metal ion molecule having a center atom and a dummy atom;

b) assigning a van der Waals radius to said center atom; and

c) assigning a charge to said dummy atom, wherein said center atom and said dummy atom are covalently bonded, and wherein said metal ion molecule has a polyhedron geometry.

2. The method of claim 1 wherein said dummy atom simulates a vacant electronic orbital of said metal ion.

3. The method of claim 1 wherein said metal ion molecule maintains its polyhedral geometry in about a nanosecond or longer protein MD simulation.

4. The method of claim 1 wherein said method is effective for use in a computer-aided protein-ligand docking simulation.

5. The method of claim 1 wherein said method is effective for use in an energy refinement.

6. The method of claim 1 wherein said method is effective for simulating the charge-transfer effect of a transition metal ion.

7. The method of claim 1 wherein said metal ion is a transition metal.

8. The method of claim 1 wherein said metal ion is a main group metal.

9. The method of claim 1 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.

10. The method of claim 1 wherein said metal ion is zinc.

11. The method of claim 1 wherein said metal ion is magnesium.

12. The method of claim 1 wherein said metal ion is calcium.

13. The method of claim 2 wherein said vacant electronic orbital imulates the lone-pair electrons of a coordination ligand of said metal ion thereby imposing an orientational requirement for a coordination ligand of said metal ion.

14. The method of claim 13 wherein said method is effective for maintaining said polyhedron geometry of said metal ion in organic and inorganic molecules in a nanosecond or longer MD simulation.

15. The method of claim 13 wherein said method is effective for use in a computer-aided protein-ligand docking simulation.

16. The method of claim 13 wherein said method is effective for use in a computer aided energy refinement.

17. The method of claim 13 wherein said method is effective for simulating charge transfer effects of transition metal ions.

18. The method of claim 17 wherein said transition metal is selected from the group consisting of zinc, cadmium, and mercury.

19. A method for performing nanosecond or longer MD simulations comprising the steps of:

a) assigning the force field parameters of Table 1 to a metal ion; and

b) performing a nanosecond or longer MD simulation.

20. The method of claim 19 wherein said method is effective for use in a computer-aided molecular dynamics simulation.

21. The method of claim 20 wherein said method is effective for maintaining a polyhedron geometry of a metal ion coordination complex containing two metal ions.

22. The method of claim 19 wherein said method is effective for use in an energy refinement of a zinc binding protein.

23. A method for performing nanosecond or longer MD simulations comprising the steps of:

a) assigning the force field parameters of Table 2 to a metal ion; and

b) performing a nanosecond or longer MD simulation.

24. A method for performing nanosecond or longer MD simulations comprising the steps of:

a) assigning the force field parameters of Table 3 to a metal ion; and

b) performing a nanosecond or longer MD simulation.

25. The method of claim 1 wherein said dummy atom has a charge ranging from about +0.1 to about +3.

26. The method of claim 1 wherein said dummy atom has a charge of about +0.5.

27. The method of claim 1 wherein said dummy atom has a charge of about +0.3333.

28. The method of claim 27 wherein said dummy atom has Lennard-Jones parameters of zero ($r^*=0$ & $e=0$).

29. The method of claim 28 wherein said metal ion is selected from the group consisting of cobalt, zinc, calcium, mercury, and magnesium.

30. The method of claim 1 wherein said metal ion is a transition metal.

31. The method of claim 1 wherein said metal ion is zinc.

32. The method of claim 19 wherein said metal ion is zinc.

33. The method of claim 1 wherein said method is used to develop a pharmaceutical drug.

34. The method of claim 19 wherein said method is used to design transcription factors used in gene therapy.

35. The method of claim 1 wherein a covalent bond between dummy atoms can be used to avoid drastic deformation of the geometry of said metal ion molecule in computer-aided energy minimizations.

36. The method of claim 1 wherein said dummy atom is located at an apex of a polyhedron.

37. A simulated metal ion molecule for use in a molecular dynamics simulation comprising a center atom having a van der Waals radius greater than zero covalently linked to one or more dummy atoms having a van der Waals radius of about zero, wherein the overall charge of said metal ion molecule is evenly distributed among said dummy atoms and wherein said center atom has a charge of zero.

38. The simulated metal ion molecule of claim 37 wherein said dummy atom has a mass of about 0.1.

39. The simulated metal ion molecule of claim 37 wherein said dummy atom has a mass greater than about 0.1.

40. The simulated metal ion molecule of claim 37 wherein said dummy atoms are located at the apices of a polyhedron.

41. The simulated metal ion molecule of claim 40 wherein said center atom is located at the center of said polyhedron.

42. The simulated metal ion molecule of claim 40 wherein said polyhedron is selected from the group consisting of trigonal, tetrahedron, pentahedron, hexagonal, septagonal, and octahedral.

43. The simulated metal ion molecule of claim 41 wherein said polyhedron is a tetrahedron.

44. The simulated metal ion molecule of claim 37 wherein said metal ion is selected from a main group or transition metal.

45. The simulated metal ion molecule of claim 37 wherein said metal ion is selected from the group consisting of zinc, cadmium, mercury, copper, nickel, cobalt, iron, manganese, calcium, and magnesium.

46. The simulated metal ion molecule of claim 37 wherein said metal ion is zinc.

47. The simulated metal ion molecule of claim 41 wherein said metal ion is zinc.

48. The simulated metal ion molecule of claim 37 wherein said metal ion is magnesium.

49. The simulated metal ion molecule of claim 37 wherein said metal ion is calcium.

50. The simulated metal ion molecule of claim 37 wherein said metal ion has a calculated energy of solvation about equal to an experimentally determined energy of solvation for said metal ion.

51. The simulated metal ion molecule of claim 50 wherein said calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.

52. The simulated metal ion molecule of claim 37 wherein said dummy atom has a charge of about 0.5.

53. The simulated metal ion molecule of claim 37 wherein said dummy atom has a charge of about 0.3333.

54. The simulated metal ion molecule of claim 37 wherein said dummy atom has a charge ranging from about $^{+}0.1$ to about $^{+}3$.